

Comment on “Anisotropic s -wave superconductivity: comparison with experiments on MgB_2 ” [A. I. Posazhennikova, T. Dahm and K. Maki, cond-mat/0204272; submitted to *Europhys. Lett.*]

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Abstract. – An analytical result for the renormalization of the jump of the heat capacity $\Delta C/C_N$ by the anisotropy of the order parameter is derived within the framework of the very recent model proposed by Posazhennikova, Dahm and Maki [cond-mat/0204272 submitted to *Europhys. Lett.*], for both oblate and prolate anisotropy. The graph of $\Delta C/C_N$ versus the ratio of the gaps on the equator and the pole of the Fermi surface, Δ_e/Δ_p , allows a direct determination of the gap anisotropy parameter Δ_e/Δ_p by fitting data from specific heat measurements $\Delta C/C_N$. Using the experimental value $\Delta C/C_N = 0.82 \pm 10\%$ by Wang, Plackowski, and Junod [*Physica C* **355** (2001) 179] we find $\Delta_e/\Delta_p \approx 4.0$.

In a very recent e-print Posazhennikova, Dahm and Maki [1] discuss a model for the gap anisotropy in MgB_2 , a material which has attracted a lot of attention from condensed matter physicists in the past two years. A central issue in this work [1] is to propose an analytic model for analyzing thermodynamic behavior. Assuming a spherical Fermi surface, a simple gap anisotropy function is suggested, $\Delta(\mathbf{k}) = \Delta_e/\sqrt{1 + Az^2}$, where $z = \cos \theta$, and θ is the polar angle. This model leads to useful results for the temperature dependence of the upper critical field H_{c2} and of the specific heat, which can be fitted to the experimental data, thereby determining the optimal anisotropy parameter A . Note that $A = (\Delta_e/\Delta_p)^2 - 1$, with $\Delta_p = \Delta(z = 1)$ and $\Delta_e = \Delta(z = 0)$, and the gap ratio is parameterized as $\Delta_e/\Delta_p = \sqrt{1 + A} > 0$.

The aim of the present Comment is to provide a convenient analytical expression giving the possibility for determining Δ_e/Δ_p from the available data for the jump of the specific heat [2]. For the latter we derive the explicit formula

$$\frac{\Delta C}{C_N} = \frac{12}{7\zeta(3)} \frac{1}{\beta_\Delta}, \text{ where } \frac{1}{\beta_\Delta} = \frac{\langle |\Delta_{\mathbf{k}}|^2 \rangle^2}{\langle 1 \rangle \langle |\Delta_{\mathbf{k}}|^4 \rangle}, \quad \langle f(\mathbf{k}) \rangle = 2 \sum_b \int \delta(\varepsilon_{b,\mathbf{k}} - E_F) f(\mathbf{k}) \frac{d\mathbf{k}}{(2\pi)^3}, \quad (1)$$

E_F is the Fermi energy, $\varepsilon_{b,\mathbf{k}}$ are the band energies, $\langle 1 \rangle$ is the density of states, ζ is the Riemann zeta function, β_Δ is analogous to Abrikosov’s parameter β_A [3], and $12/7\zeta(3) = 1.42613\dots$ is the sacramental BCS ratio. Then

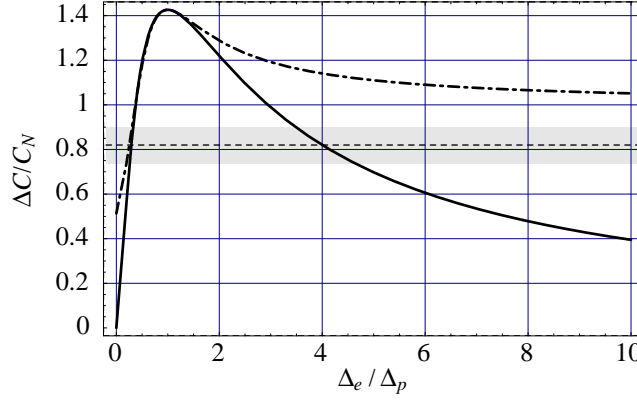


Fig. 1 – Jump of the specific heat $\Delta C/C_N$ versus the “equatorial-to-polar” gap ratio Δ_e/Δ_p . For a given $\Delta C/C_N$ value we have oblate $\Delta_e/\Delta_p > 1$ and prolate $\Delta_e/\Delta_p < 1$ solutions. The solid line gives our present analytical result eq. (2) for the model by Posazhennikova, Dahm and Maki [1]. The dash-dotted line is our analytical solution [5] for the model by Haas and Maki [4]. The dashed line is the jump ratio $\Delta C/C_N = 0.82 \pm 10\%$ measured by Wang, Plackowski, and Junod [2], with the shaded area showing the experimental error bar.

following the weak-coupling BCS approach [1,4] we derived the explicit analytic expressions valid for $A > 0$, and $-1 < A < 0$, respectively

$$\frac{\Delta C(A)}{C_N} = \begin{cases} \frac{12}{7\zeta(3)} \frac{2(1+b^2)(\arctan b)^2}{b^2 + b(1+b^2)\arctan b}, & b = \sqrt{A} = \sqrt{\left(\frac{\Delta_e}{\Delta_p}\right)^2 - 1}, \\ \frac{12}{7\zeta(3)} \frac{2(1-p^2)(\tanh^{-1} p)^2}{p^2 + p(1-p^2)\tanh^{-1} p}, & p = ib = \sqrt{-A} = \sqrt{1 - \left(\frac{\Delta_e}{\Delta_p}\right)^2}. \end{cases} \quad (2)$$

For a given specific heat jump, this expression leads to *two* solutions (oblate, $\Delta_e/\Delta_p > 1$, and prolate, $\Delta_e/\Delta_p < 1$). The relevant example is shown in fig. 1; the function $\Delta C(A)/C_N$ is tabulated in ref. [1]. The analysis of the angular dependence of H_{c2} [6,7] performed in the commented paper [1] unambiguously demonstrates that one has to analyze only the “oblate” case. Thereby the experimentally reported value in ref. [2] $\Delta C/C_N = 0.82 \pm 10\%$ gives $A \approx 16$ and $\Delta_e/\Delta_p \approx b \approx 4.0 \pm 10\%$. For this significant anisotropy, the “distribution” of Cooper pairs $\langle |\Delta_{\mathbf{k}}|^2 \rangle \propto 1/[k_z^2 + (k_F/b)^2]$ has a maximum at $k_z = 0$. This general qualitative conclusion is in agreement with the hints from band calculations that the maximal order parameter is concentrated in an almost two-dimensional electron band, but all bands $\varepsilon_{b,\mathbf{k}}$ take part in the normal specific heat per unit cell $C_N = (\pi^2/3)k_B^2 T \langle 1 \rangle$.

For the two-band model, advocated for the first time for MgB_2 in ref. [8], eq. (1) gives (to within a typographical correction) the result by Moskalenko [9]

$$\frac{\Delta C}{C_N} = \frac{12}{7\zeta(3)} \frac{(|\Delta_1|^2 \rho_1 + |\Delta_2|^2 \rho_2)^2}{(\rho_1 + \rho_2)(|\Delta_1|^4 \rho_1 + |\Delta_2|^4 \rho_2)} = 1.426 \frac{[z^2 x + (1-x)]^2}{z^4 x + (1-x)}, \quad \text{where } z = \frac{\Delta_1}{\Delta_2}, \quad x = \frac{\rho_1}{\rho_1 + \rho_2}, \quad (3)$$

and ρ_1 and ρ_2 are the densities of states for the two bands. Taking for an illustration $x = 0.515$ and $\Delta C/C_N = 0.82$, eq. (3) gives $\Delta_1/\Delta_2 \approx 4.0$ in agreement with $\Delta_e/\Delta_p \approx 4.0$ obtained using eq. (2). Thus the gap ratios are model-independent. For a survey on a set of parameters see Table I in ref. [10]. Certainly the jump of the heat capacity alone cannot be an arbiter for the validity of any model, so subtleties, e.g., related to strong coupling effects and other anisotropies, can be hidden in the parameters spread in the table mentioned.

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